Journal of Quantitative Spectroscopy & Radiative Transfer 161 (2015) 157–170

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

Atomic structure calculations and identification of EUV and SXR spectral lines in Sr XXX

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ARTICLE INFO

Article history:
Received 23 January 2015
Received in revised form
13 April 2015
Accepted 16 April 2015
Available online 25 April 2015

Keywords:
Energy levels
Spectral lines
Extreme Ultraviolet
Soft X-ray
Wavelengths
Radiative data

ABSTRACT

We report an extensive theoretical study of atomic data for Sr XXX in a wide range with L-shell electron excitations to the M-shell. We have calculated energy levels, wave-function compositions and lifetimes for lowest 113 fine structure levels and wavelengths of an extreme Ultraviolet (EUV) and soft X-ray (SXR) transitions. We have employed multi-configuration Dirac Fock method (MCDF) approach within the framework of Dirac–Coulomb Hamiltonian including quantum electrodynamics (QED) and Breit corrections. We have also presented the radiative data for electric and magnetic dipole (E1, M1) and quadrupole (E2, M2) transitions from the ground state. We have made comparisons with available energy levels compiled by NIST and achieve good agreement. But due to inadequate data in the literature, analogous relativistic distorted wave calculations have also been performed using flexible atomic code (FAC) to assess the reliability and accuracy of our results. Additionally, we have provided new atomic data for Sr XXX which is not published elsewhere in the literature and we believe that our results may be beneficial in fusion plasma research and astrophysical investigations and applications.

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1. Introduction

In few past decades, EUV and SXR transitions are in particular astrophysical interest. They provide elaborate

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http://dx.doi.org/10.1016/j.jqsrt.2015.04.009
0022-4073/

information about coronal atmosphere. The energy emitted by the sun lies within the region of EUV (50–1200) Å and SXR (1–50) Å are necessary and prominent keys of physical phenomenon in Earth's upper atmosphere and ionosphere. In the past, EUV rays radiated from different kind of elements have examined and diagnosed in a methodical manner in fusion devices by implementing the technique of laser blow-off and the impurity pellet injection [1,2]. After the technical improvement over a number of years, two EUV spectrometers of wavelength ranges 10–130 Å and 50–500 Å have been installed in LHD as impurity monitor [3,4] and recently a space resolved EUV spectrometer of wavelength ranges 60–400 Å is developed [5].

During the last few years high Z ion spectra have become the subject of real research and a remarkable work in experimental as well as in the theoretical side on neutral and highly ionized strontium ions has been studied [6–14]. Maximum number of lines emitted from high Z ions lay within the region of EUV and SXR. The main target of the analyses is wavelength identification. Since the comprehensive and detailed study on the identification of wavelengths of spectral lines is necessary for high Z ions and therefore, in the present paper, we theoretically identified the EUV and SXR transitions and plotted the Sr XXX spectra within the SXR.

In the past, several experimental measurements and theoretical calculations on highly ionized F-like Sr ion have been performed using several techniques. Early, Cheng et al. [15] has provided E1, E2 and M1 transition energies, oscillator strengths, line strengths and radiative rates for many ions including the F-like Sr using the MCDF method. The SXR spectral lines for various transitions of highly ionized ions including Sr XXX is reported by using a laser produced plasma technique [16–18]. Ivanova and Glushkov [19] computed splitting between the first three levels for various F-like ions (including Sr XXX) by applying relativistic perturbation theory. The transition probabilities for Sr XXX and other ions using scaled radial integrals or the Dirac–Fock method has been listed by Kaufman and Sugar [20]. Further, a fully relativistic calculation of E1 oscillator strengths and collision strengths of Sr XXX for lowest three levels was performed by applying relativistic distorted wave method by Sampson et al. [21]. A significant data of ionization potentials and binding energies for Sr XXX and other ions were also presented in the literature [22–24]. Gu [25] computed the energies of $1s^2 2l^q$ $(1 \le q \le 8)$ for ions with nuclear charge up to 60 using combined approach of configuration interaction and Many Body Perturbation Theory (MBPT). Recently, Sansonetti [26] tabulated energy levels, transition probabilities and transition energies for the spectra of strontium ions upto Sr XXXVIII. More recently, Jönsson et al. [27] computed energies, radiative rates and oscillator strengths for transitions within $2s^2 2p^5$ and $2s2p^6$ for Si VI to W LXVI using the MCDF and relativistic configuration interaction (RCI) method.

Inspite of the publishing of various papers related to Sr XXX, there is a scarcity of complete, consistent and accurate atomic data for higher levels of this ion in the literature. Therefore, in the present work we report the results of energy levels and lifetimes for all levels of $2s^2 2p^5$, $2s2p^6$, $2s^2 2p^4 3l$, $2s2p^5 3l$ and $2p^6 3l$ (l=s, p, d) configurations along with oscillator strengths and transition probabilities for E1, E2, M1 and M2 multipole transitions from the ground state for Sr XXX. QED corrections due to vacuum polarization and self energy effects and Breit correction due to the exchange of virtual photons between two electrons are fully considered. We have identified a EUV transition and 108 SXR transitions from the ground state to higher excited levels in F-like Sr and plotted SXR spectra of Sr XXX for allowed transitions. The present calculations may be helpful for examining new data from fusion plasma and astrophysical sources.

2. Theoretical method

To perform these large-scale calculations, fully relativistic MCDF method revised by Norrington [28] formerly developed by Grant et al. [29] is applied which has been successfully applied in our previous work [30–34]. It comprises contributions from Breit interactions as well as QED corrections as a first order perturbation theory. Since the detailed explanation of this method has been presented elsewhere [29,35–38], so only a brief outline is discussed here. We have employed the extended average level (EAL) scheme to obtain radial wave functions at the time of self consistent field (SCF) calculations in which weighted trace of the Hamiltonian matrix is minimized. For N electron atom or ion, Dirac–Coulomb Hamiltonian in MCDF method can be written as follows

$$\hat{H}^{\mathrm{DC}} = \sum_{i=1}^{N} \hat{H}_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{|\hat{r}_i - \hat{r}_j|} \tag{1}$$

where $\hat{H}$, the one electron Hamiltonian is given by

$$\hat{H}_i = c\vec{\alpha}_i.\vec{p}_i + \beta mc^2 + V_{\mathrm{nuc}} \tag{2}$$

In Eq. (2) first two terms denote kinetic energy of an electron and the last term represents the Coulomb potential of the nucleus. α and β are 4×4 Dirac matrices and c is the speed of light.

The N-electron wave functions, the sum of products of central-field Dirac orbitals in matrix form is defined as follows:

$$\varphi_{\mathrm{nkm}} = \frac{1}{r}\begin{bmatrix} P_{\mathrm{nk}}(r) & \chi_{\mathrm{km}}(\theta,\varphi,\sigma) \\ -iQ_{\mathrm{nk}}(r) & \chi_{-\mathrm{km}}(\theta,\varphi,\sigma) \end{bmatrix} \tag{3}$$

where Q_{nk}(r) and $P_{\mathrm{nk}}(r)$ are large and small components of one electron radial wavefunctions. $k = \pm(j+1/2)$ for $l = j \pm 1/2$

k and m are the relativistic angular quantum number and m is also the projection of total angular momentum j.

The spinor spherical harmonic function is given by

$$\chi_{\mathrm{km}}(\theta,\varphi) = \sum\nolimits_{\sigma = \pm\frac{1}{2}} \langle lm - \sigma \tfrac{1}{2}\sigma \left| l\tfrac{1}{2}jm \right\rangle Y_l^{m-\sigma}(\theta,\varphi)\varphi^{\sigma} \tag{4}$$

χ_{km} has 2 components.

An atomic state function (ASF) for N electron atom or ion is built by the linear combination of n electronic